

Final report on AFOSR FA9550-07-1-0425⁰⁵⁴⁴ entitled
Novel Mathematical and Computational Techniques for
Robust Uncertainty Quantification

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This final report summarizes accomplishments in two areas of uncertainty quantification and computational probability.

1 Methods for modeling and integrating different types of uncertainty

1.1 Problem formulation and issues

Uncertainty quantification refers to a broad set of techniques for understanding the impact of uncertainties in complicated mechanical and physical systems. In this context "uncertainty" can take on many meanings. Aleatoric uncertainty refers to inherent uncertainty due to stochastic or probabilistic variability. This type of uncertainty is *irreducible* in that there will always be positive variance since the underlying variables are truly random. Epistemic uncertainty refers to limited knowledge we may have about the model or system. This type of uncertainty is *reducible* in that if we have more information, e.g., take more measurements, then this type of uncertainty can be reduced. For many problems where uncertainty quantification is important, the acquisition of data is difficult or expensive. The epistemic uncertainty cannot be removed entirely, and so one needs modeling and computational techniques which can also accommodate this form of uncertainty.

However, in most applications it is (perhaps implicitly) assumed that epistemic uncertainty can be modeled by aleatoric uncertainty. One reason is purely based on convenience in that, at least as they have been developed to date, most computational techniques (e.g., polynomial chaos and Monte Carlo) are based on the assumption that the user can identify some "appropriate" distribution for each uncertain aspect of the system, regardless of the type of uncertainty, aleatoric or epistemic. If one is interested in just basic qualitative properties of the system then this may not be a central issue, since virtually any model of uncertainty will give information on the sensitivities of the system. However, when the intended use of uncertainty quantification is for regulatory assessment or some other application where performance measures are sensitive to distributional assumptions, the issue becomes much more important, and one should carefully distinguish how one accounts for the two types of uncertainty.

Hence important issues are: (i) how should one model uncertainties that are not of the aleatoric type, and (ii) can one work with the resulting formulation from a numerical perspective.

1.2 Results and key findings

In the paper [1] we develop an approach that (i) logically distinguishes those aspects of uncertainty that are treated as stochastic variability from other forms of uncertainty, (ii) in cases where a stochastic model is theoretically valid but for which determination of the distribution is not practical, gives bounds for performance measures that are valid for explicitly identified families of distributions, and (iii) is computationally feasible if ordinary uncertainty propagation is feasible. The different forms of uncertainty that are covered by the formulation include: (a) aleatoric with known distribution; (b) aleatoric with partly known distribution (mingled aleatoric and epistemic); (c) epistemic for which one is willing to model by a family of aleatoric uncertainties, and (d) epistemic where one is only willing to place bounds on the uncertainties.

Suppose that random variables with a *known* distribution will take values in a Polish space \mathcal{X} . Variables whose distribution is *not known* or are otherwise of the epistemic variety take values in the space \mathcal{Y} . Let the performance measure of interest for some given problem is assumed to be of the form

$$\int_{\mathcal{X}} \int_{\mathcal{Y}} F(x, y) \gamma(dy) \mu(dx),$$

where μ (resp., γ) is a probability measure on \mathcal{X} (resp., \mathcal{Y}). If X and Y are independent random variables with distributions μ and γ , then $F(X, Y)$ represents both the performance measure (e.g., a second moment) as well as the underlying physical or mechanical system that maps these aleatoric and epistemic inputs into outputs.

It is known that risk-sensitive performance measures can be used to produce performance bounds that are robust with respect to the underlying distributions. The standard risk-sensitive performance measure is

$$\Lambda_c = \frac{1}{c} \log \int_{\mathcal{X}} \int_{\mathcal{Y}} e^{cF(x, y)} \gamma(dy) \mu(dx).$$

Neither of these measures differentiate the variables according to type (aleatoric or epistemic) and given that the performance measure of interest is actually F , the use of a risk-sensitive version of the cost is not well motivated for the aleatoric variables. Indeed, use of this measure will give bounds that are robust with respect to variations on a distribution that is known, and obviously such bounds will not be as tight as possible.

In [1] two hybrid risk-sensitive measures are introduced, as well as variations. To simplify we mention only the theory developed for the (more

useful) form

$$\Lambda_c^1 = \frac{1}{c} \log \int_{\mathcal{Y}} e^{\int_{\mathcal{X}} cF(x,y)\mu(dx)} \gamma(dy).$$

Using the relative entropy representation for exponential integrals, it follows that for any distribution $\theta(dy)$

$$\int_{\mathcal{Y}} \int_{\mathcal{X}} F(x,y)\mu(dx)\theta(dy) \leq \frac{1}{c} R(\theta(dy) \parallel \gamma(dy)) + \Lambda_c^1.$$

This gives a bound on the performance measure for an arbitrary distribution on Y , but with the distribution on X equal to the known true distribution. The distributions thus play very different roles. In particular, we think of γ as a *nominal* distribution of Y , which should be distinguished from a possible *true* distribution. The risk sensitive functional Λ_c^1 , whose numerical evaluation can be carried out by a variety of methods (in [1] we use polynomial chaos), is based on the nominal distribution. Through the relative entropy duality, it yield various bounds (depending on c) on a families of distributions, with the relative entropy distance the key metric.

Suppose that a bound on performance over a specific family of distributions is needed. Let R^* denote the maximum of relative entropy with respect to the nominal model over this family that we wish to allow. Then the *tightest possible bound* is obtained by minimizing

$$\Lambda_c^1 + \frac{1}{c} R^*$$

over $c > 0$. Thus given a prescribed uncertainty in the epistemic variables, one can compute a bound on the performance over all distributions in the family and which holds with equality for at least one. This optimizing c , which exists and is unique, can be computed using the same techniques used to compute the performance measure itself. We show in [1] that this function has only one local minimum over $c \in (0, \infty]$, and thus the global minimum is easy to compute.

In [1] examples of various types and numerical data is presented, as well as the corresponding theory where all that is assumed regarding the epistemic variables is that they are constrained to some given set. The use of polynomial chaos methods for the evaluation of the risk-sensitive functionals is developed, and explicit relative entropy distances for common families of distributions are listed.

Two additional papers on this topic are in preparation, both with Kenny Chowdhary, a graduate student in the department. One is concerned with optimization in the presence of both epistemic and aleatoric uncertainties, and the second is concerned with estimation in this same framework.

2 Computational methods for rare event problems

2.1 Problem formulation and issues

There is significant interest in the application of uncertainty quantification to problems with small probabilities (rare events). For example, it is a research focus for the SAMSI/Sandia Summer School on Uncertainty Quantification in 2011. Though these probabilities may be small, they are often critical measures of system performance and one needs reasonably reliable numerical methods. Unfortunately, standard numerical schemes are not at all reliable for problems with rare events.

This part of the research project was concerned with developing efficient Monte Carlo algorithms for rare event simulation and the associated large deviations theory. There are two methods currently in use. One is based on simulating according to a different distribution and then correcting for any induced bias via the likelihood ratio (importance sampling). The key question here is how to select the new sampling distribution. The second method simulates a branching process, i.e., collection of particles that can split according to certain rules to form new particles, each of which behaves like the original particle or process. The splitting rules are designed to make the rare event likely for at least one of the descendent particles, and the estimator is the ratio of number of particles for which the rare outcome is observed to the total number of descendents. The key question here is what should trigger a split and, given that a split occurs, the number of descendents. Most of the literature on these methods features schemes based on heuristic design, with little or no analysis. However, the design problem with both methods is subtle, and reasonable looking schemes can perform quite poorly. Indeed, simulations based on improperly designed schemes could be highly misleading.

A second class of problems considers the numerical approximation of the invariant distribution for stochastic systems with multiple metastable states using the occupation measure of a related Markov process. Moving from one metastable state to another is a rare event, and its treatment is the key question in the design of efficient Monte Carlo schemes. There are many ad hoc algorithms available. However, these algorithms do not always work well and have to be applied with some care.

2.2 Results and key findings

In prior work we demonstrated that the design of a reliable and high performing important sampling scheme would follow if one could construct a

subsolution to a related Hamilton-Jacobi-Bellman equation (a partial differential equation). Moreover, we showed that the existence of such a subsolution is in some sense necessary. The paper [4] considers the analysis of the “weighted-serve-the-longer-queue” policy. Such service policies are common, and in particular a variant is frequently used in wireless communication. The goal of the importance sampling scheme is to accurately estimate probabilities associated with buffer overflows and delays, which are critical performance measures. The model is fairly complex, since the policy introduces a kind of discontinuous behavior into the stochastic evolution. We showed how the approach based on subsolutions to a related Hamilton-Jacobi-Bellman equation developed in previous papers could be adapted to deal with such complicated process dynamics.

The paper [2] analyzes a number of branching type schemes, including RESTART (REpetitive Simulation Trials After Reaching Thresholds) and DPR (Direct Probability Redistribution). It is established that the design of a stable (namely, controlled number of particles) and asymptotically optimal (namely, tightly controlled variance) splitting algorithms can be achieved by constructing suitable viscosity subsolutions to a Hamilton-Jacobi-Bellman (HJB) equation. This HJB equation is in fact the same one in importance sampling analysis. This is a useful theoretical result, since it indicates that the construction of subsolutions is in any case a central aspect to solving the numerical problem.

A much more complex algorithm can be based on what is called an *interacting particle system*. The paper [3] provides the first rigorous analysis of the performance of this class of algorithms in the small probability limit. Owing to the complexities of the algorithm, the analysis is limited to dimension one. However, the results support some of the claims that have been made concerning these algorithms (but based only on numerical evidence), and in particular that, at least for one dimensional problems, they are less sensitive to the details of the underlying distributions than competing schemes.

The paper [5] considers the problem of approximating stationary distributions of a Markov chain by simulation. Our initial goal was to use large deviation ideas to choose design parameters in an existing scheme known as parallel tempering. Parallel tempering (also known as replica exchange sampling) is a standard method for simulating complex systems, and is used in many commercial software packages. In this algorithm simulations are conducted in parallel for a family of Markov chains indexed by a “temperature” parameter, and the key improvement over standard Monte Carlo is a swap mechanism that exchanges configurations between these parallel simulations

at a given rate. The mechanism is designed to allow the low temperature system to escape from deep local energy minima where it might otherwise be trapped, via those swaps with the higher temperature components. Based on large deviation theory, we have argued that the rate of convergence of the empirical measure is a monotone increasing function of the swap rate. This suggests that one should raise the swap frequency in order to improve efficiency, but this is eventually counter-productive since eventually most of the computational effort is directed towards swapping and little towards moving the process dynamics. However, it turns out that one can construct a simulation scheme that is equivalent to the limit of the parallel tempering schemes in the sense of distributions, but which involves no swapping at all. With this scheme, which we call *infinite swapping* (INS), the effect of the swapping is captured by a collection of weights that influence both the dynamics and the empirical measure.

While the infinite swapping scheme optimizes the convergence rate as described above, it has practical limitations in implementation due to the complexity of the weights when the number of temperatures is large (>7). Complex problems often involve scores of temperatures, and so it was critical to overcome this limitation. We have developed an approximation to the full infinite swapping which is based on alternating between *partial infinite swapping* (PINS) algorithms, which can be shown to approximate (theoretically and practically) the INS scheme. The mathematical theory for the INS and PINS is developed in [5]. Numerical studies on fairly complex Lennard-Jones systems (very challenging benchmark problems from chemistry) have been conducted. Improvements of three orders of magnitude in performance over conventional parallel tempering were observed at an increased computational cost of 5-15%.

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- Prof. Paul Dupuis
- Dr. Alex Solomonoff, Postdoctoral researcher
- Dr. Xie Li, Postdoctoral researcher
- Yi Cai, Graduate student
- Sirui Tan, Graduate student
- Kenny Chowdharry, Graduate student

4 Preprints and publications

1. Distinguishing and integrating aleatoric and epistemic variation in uncertainty quantification, K. Chowdhary and P. Dupuis, submitted to *ESAIM*.
2. The design and analysis of a generalized RESTART/DPR algorithm for rare event simulation, T. Dean and P. Dupuis, *Ann. Oper. Res.*, DOI 10.1007/s10479-009-0664-7.
3. Analysis of an interacting particle method for rare event estimation, Y. Cai and P. Dupuis, *preprint*.
4. Importance sampling for weighted-serve-the-longest-queue, P. Dupuis, K. Leder and H. Wang, *Math. of Oper. Res.*, **34**, (2009), 642–660.
5. On the infinite swapping limit for parallel tempering, P. Dupuis, Y. Liu, H. Wang, J. D. Doll and H. Plattner, to be submitted to *SIAM J. on Multiscale Simulation*.
6. Stochastic comparison, boundedness, weak convergence, and ergodicity of a random Riccati equation with Markovian binary switching, L. Xie, under revision for *SIAM J. On Control and Optimization*.
7. Inverse Lax-Wendroff procedure for numerical boundary conditions of conservation laws, S. Tan and C.-W. Shu, *J. of Comp. Phys.*, **229**, (2010), 8144–8166.
8. A high order moving boundary treatment for compressible inviscid flows, S. Tan and C.-W. Shu, *J. of Comp. Phys.*, **230**, (2011), 6023–6036.

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